

A factorization algorithm to compute Pfaffians

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Abstract

We describe an explicit algorithm to factorize an even antisymmetric N^2 matrix into triangular and trivial factors. The construction resembles the Crout algorithm for LU factorization. It allows for a straight forward computation of Pfaffians (including their signs) at the cost of $N^3/3$ flops.

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Pfaffians play a role in statistical physics as well as in quantum field theories (QFT) related to particle physics. They are defined for antisymmetric even-sized quadratic matrices A with elements $a_{ij} \in \mathbb{C}$ and $i, j = 1, \dots, N = 2n$. As basic definition we take

$$\text{Pf}(A) = \frac{1}{2^n n!} \sum_{\pi \in S_N} \text{sgn}(\pi) a_{\pi(1)\pi(2)} a_{\pi(3)\pi(4)} \cdots a_{\pi(N-1)\pi(N)}, \quad (1)$$

a sum over permutations in the symmetric group of N elements reminiscent of the definition of determinants. In the path integral formulation of QFT one encounters Gaussian Grassmann integrals [1] for Majorana fermions of the form

$$\int D\xi e^{-\frac{1}{2}\xi^\top A \xi} = \text{Pf}(A). \quad (2)$$

Here the components $\xi_i, i = 1, \dots, N$ carry indices that stand for a compound labeling a Euclidean lattice site x and a Dirac spinor component. The identity follows from the rules of Grassmann integration with $D\xi$ being a product over all differentials ordered such that the sign works out. In applications like [2] the antisymmetric matrix $A = \mathcal{C}(\not{D} + m)$ is built from charge conjugation \mathcal{C} and a (lattice) Dirac operator \not{D} . It may depend on other fields such as a scalar field ($m \rightarrow m + \varphi(x)$) for the Gross Neveu model [3], [4]. Majorana fermions and Pfaffians appear almost unavoidably in formulations of supersymmetric models, see [5] for an early attempt of a lattice simulation as well as [6] for more recent results.

Up to a *nontrivial* sign a Pfaffian is the square root of a determinant. This may be shown by doubling the Majorana fermion (2) into a Dirac fermion

$$[\text{Pf}(A)]^2 = \int D\xi D\xi' e^{-\frac{1}{2}(\xi^\top A \xi + \xi'^\top A \xi')} = \int D\psi D\bar{\psi} e^{-\bar{\psi} A \psi} = \det(A) \quad (3)$$

with $\psi = (\xi + i\xi')/\sqrt{2}$, $\bar{\psi} = (\xi - i\xi')^\top/\sqrt{2}$ and a corresponding definition of $D\psi D\bar{\psi}$. If we choose the Majorana representation for the Dirac matrices, then A is manifestly real. Then there is a pseudofermion representation for each degenerate fermion pair¹

$$[\text{Pf}(A)]^2 = [\det(A^2)]^{1/2} = \int D\varphi e^{-\frac{1}{2}\varphi^\top (A^2)^{-1} \varphi} \quad (4)$$

in terms of real bosonic variables φ which can be a starting point of a hybrid Monte Carlo simulation as in [3].

For smaller systems, in particular in two dimensions and for algorithmic investigations, it can be of interest to compute Pfaffians and determinants exactly in

¹Note that this is not suitable to simulate a single Dirac fermion, if its Majorana components are mixed by non-real interactions.

simulations [7], [8] and for other purposes [2], even if practicable algorithms cost proportional to N^3 . As the sign of the Pfaffian cannot be obtained from algorithms for determinants we find it of some interest to describe in this letter² an algorithm for the Pfaffian itself. Gaussian elimination schemes suitably adapted to antisymmetric matrices are described in [9] and are also mentioned or contained in the deeper layers of algorithms described in recent works requiring the computation of Pfaffians [6], [10], [11], [12]. The recursive factorization formulae worked out below are to our knowledge however not in the literature in this easily programmable explicit form.

For a nonsingular antisymmetric A there exists a factorization of the form

$$A = PJP^\top \quad (5)$$

where P is lower triangular. The trivial antisymmetric matrix J with $\text{Pf}(J) = 1$ has antisymmetric 2×2 blocks around the diagonal. Its nonzero elements are enumerated by

$$J_{ii-(-1)^i} = -(-1)^i, \quad i = 1, 2, \dots, N. \quad (6)$$

We have learned (5) in [5] where it is attributed to [13]. In the form of our algorithm we below give a constructive proof for it. With the factorization given, we may change variables in the Grassmann integral (2) $P^T \xi = \eta$ with the Jacobian³ $D\xi = \det(P)D\eta$ and, proving in passing another well-known relation, we obtain

$$\text{Pf}(A) = \det(P) \int D\eta e^{-\frac{1}{2}\eta^\top J \eta} = \det(P) \text{Pf}(J) = \prod_{i=1}^N p_{ii}. \quad (7)$$

The factorization (5) will be constructed in a way similar to the Crout algorithm for the LU factorization [14] of general matrices. The matrix P has more independent entries than A , but the factorization is rendered unique by setting for all *odd* i

$$p_{ii} = 1, \quad p_{i+1i} = 0, \quad i = 1, 3, 5, \dots, N-1 \quad (8)$$

beside having $p_{ij} = 0$ for $i < j$.

The basic idea of the algorithm is to write out (5) in components in a special order by considering for $i = 1, 3, 5 \dots$ the pairs

$$p_{ji+1} = a_{ij} - \sum_{k=1}^{i-2'} (p_{ik}p_{jk+1} - p_{ik+1}p_{jk}), \quad j = i+1, i+2, \dots, N, \quad (9)$$

$$(-p_{i+1i+1})p_{ji} = a_{i+1j} - \sum_{k=1}^{i-2'} (p_{i+1k}p_{jk+1} - p_{i+1k+1}p_{jk}), \quad (10)$$

$$j = i+2, i+3, \dots, N.$$

²Based on the bachelor thesis by J.R., Humboldt university, 2009.

³Remember that the fermionic Jacobian is inverse to the bosonic one [1].

Here the primed sums over k run over *odd integers only* and (8) has been exploited. If we assume for a moment that we can always divide by p_{i+1i+1} in (10) then we may column-wise solve for the nontrivial $p_{j2}, p_{j1}, p_{j4}, p_{j3}, \dots p_{NN}$. It is decisive to note that in this order we only encounter columns of P on the right hand sides of (9), (10) that have been computed before.

Even for simple regular matrices the assumption $p_{i+1i+1} \neq 0$ may not always be fulfilled in the steps with (10). Both for this reason and to improve the numerical precision a pivoting scheme is mandatory. To that end we introduce a permutation π as in (1) and replace A, P by re-arranged copies A', P' with matrix elements

$$a'_{ij} = a_{\pi(i)\pi(j)}, \quad p'_{ij} = p_{\pi(i)j} \quad (11)$$

and note that (5) is equivalent to $A' = P'JP'^\top$ and thus ‘covariant’ under such a relabelling. We consider the above process now for A', P' with π initially set to the identity. Each time after completing (9) for some i we now determine the value j along the column where $|p'_{ji+1}|$ is maximal and denote it by j_{\max} . Before proceeding with (10) we swap the entries $\pi(i+1) \leftrightarrow \pi(j_{\max})$. It is important to note that this modification does not invalidate⁴ any of the earlier uses of (9) and (10). In this way we never divide by zero except when the whole column constructed via (9) vanishes, in which case one can show that A is singular. In all other cases we arrive at the factorization of the matrix $A' = \Pi A \Pi^\top$ where the matrix Π implements the index permutation with π . Then we obtain $\text{Pf}(A)$ from

$$\text{Pf}(A) = \det(\Pi^{-1}) \text{Pf}(A') = \text{sgn}(\pi) \prod_{i=1}^n p'_{2i2i}. \quad (12)$$

Our PJP factorization for computing the Pfaffian requires approximately $N^3/3$ flops (counting both multiplications and additions). The signum is known by counting the transpositions that went into building π .

We end by reporting on a brief test. We consider the Wilson fermion matrix on an $L \times L$ square lattice

$$A_W = c_0 \mathcal{C} \left[2 - \frac{1}{2} \sum_{\mu=0,1} \{ (1 - \gamma_\mu) \delta_{x, x - \hat{\mu}} + (1 + \gamma_\mu) \delta_{x, x + \hat{\mu}} \} \right] \quad (13)$$

which is an antisymmetric matrix with $N = 2L^2$. The Dirac matrices are given in terms of Pauli matrices, $\mathcal{C} = i\tau_2$, $\mathcal{C}\gamma_0 = \tau_1$, $\mathcal{C}\gamma_1 = \tau_3$, $\hat{\mu}$ is a unit vector in the positive μ direction, and the δ symbols here incorporate *antiperiodic* boundary

⁴This is because we have generated complete columns whose entries are permuted in the same way on both sides of the equations. The column indices of earlier columns on the other hand are untouched as $j_{\max} \geq i + 1$.

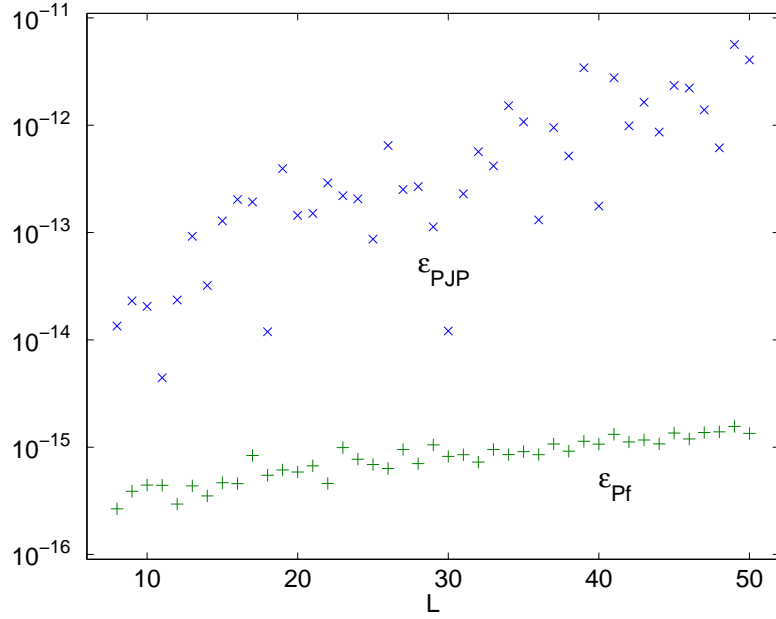


Figure 1: Precision of Pf (\times) and the factorization (+) defined in (14) as functions of the lattice size L associated with matrices of size $N = 2L^2$.

conditions in both directions thus making A_W nonsingular without a mass term. The Pfaffian for this matrix can be computed exactly by Fourier transformation [15]. To avoid a range overflow we have used this information to determine c_0 in (13) such that $\text{Pf}(A_W) = 1$ holds up to roundoff errors. We have coded the procedure described above and have run it with $L = 8, 9, \dots, 50$ in standard 64 bit precision. In Figure 1 we plot the deviations

$$\varepsilon_{\text{Pf}} = |\text{Pf}(A_W) - 1|, \quad \varepsilon_{\text{PJP}} = \|A'_W - P'JP'^\top\| \quad (14)$$

as functions of L where the matrix norm in ε_{PJP} is given by the largest singular value. We note that apart from a general trend they sometimes are exceptionally small leading to some non-uniformity with L .

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